

Supporting Information

DART-HRMS Triage Approach Part 2 – Application to the Detection of Cannabinoids and Terpenes in Recreational *Cannabis* Products

AUTHORS: Megan I. Chambers^a and Rabi A. Musah, Ph.D.^{a*}

^aDepartment of Chemistry, University at Albany – State University of New York (SUNY), 1400 Washington Avenue, Albany, NY 12222

*Corresponding Author: rmusah@albany.edu

This document contains: (1) product images of recreational *Cannabis* flower samples, with insets featuring samples of the marijuana flower; (2) DART mass spectra (collected in positive-ion mode), structures, $[M+H]^+$ chemical formulas, and corresponding protonated masses of cannabinoids known to be in *Cannabis sativa* products; (3) DART mass spectra (collected in negative-ion mode), structures, $[M-H]^-$ chemical formulas, and corresponding deprotonated masses of cannabinoids known to be in *Cannabis sativa* products; (4) DART mass spectra (collected in positive-ion mode) of the remaining edibles, capsules, and pre-rolls not featured in **Figure 3** of the main document, with photographs of the products featured in the insets; (5) DART mass spectra (collected in negative-ion mode) for all non-flower *Cannabis* products (i.e., edibles, capsules, oils, tinctures, vape products, topicals, concentrates, and pre-rolls), with photographs of the products featured in the insets; (6) table of DART mass spectral data (collected in positive-ion mode) consistent with cannabinoids and terpenes reported in the recreational *Cannabis* products; (7) table of DART mass spectral data (collected in negative-ion mode) consistent with cannabinoids reported in the recreational *Cannabis* products; (8) DART mass spectra (collected in negative-ion mode) of the recreational *Cannabis* flower samples, with photographs of the flower shown in the insets; and (9) DART mass spectra (collected in negative-ion mode) of the edible candies prepared in-house from our previous study.



Figure S1. Product images of recreational *Cannabis* flower samples, with insets featuring the samples of the marijuana flower.

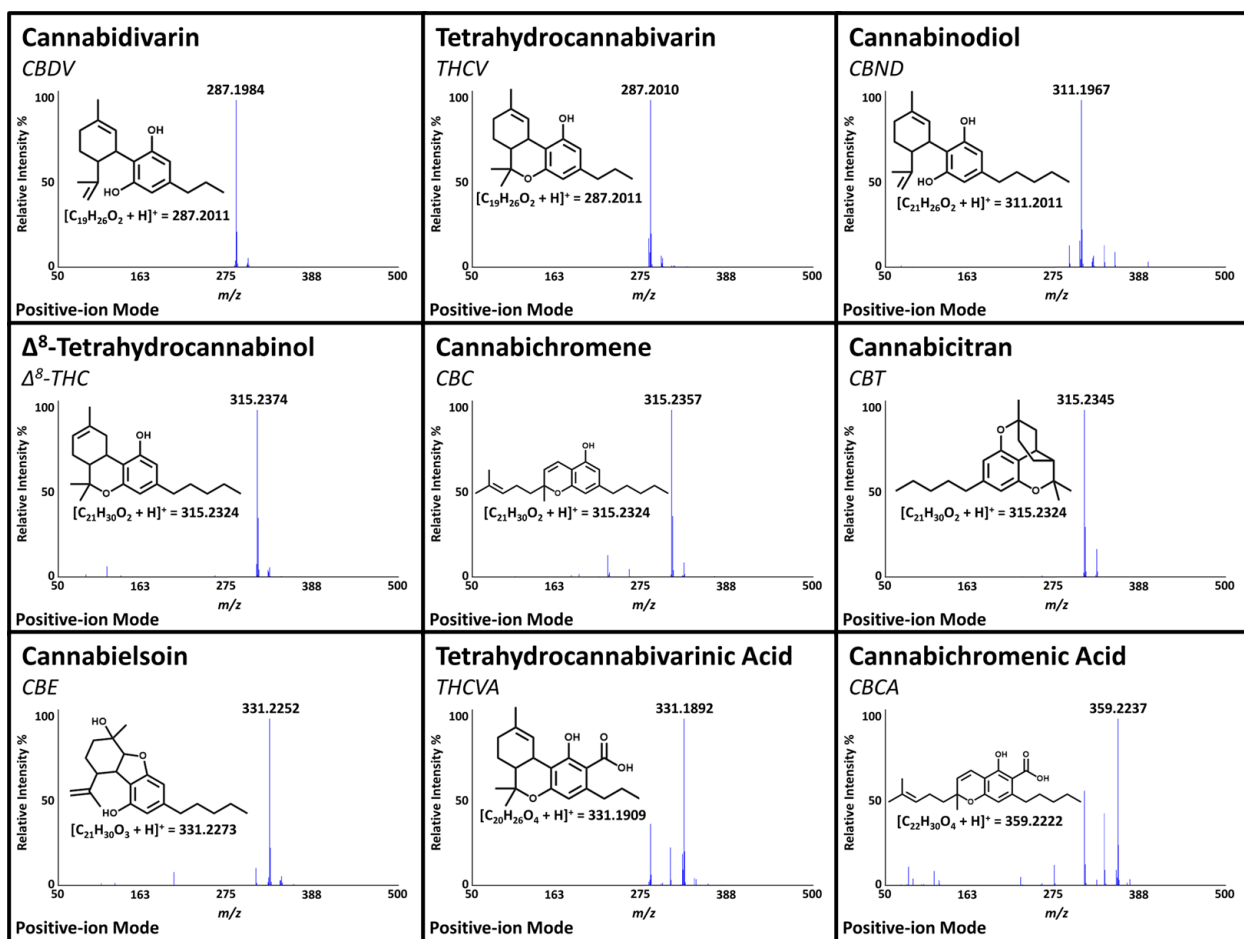


Figure S2. DART mass spectra (collected in positive-ion mode at an orifice 1 voltage of 20 V), structures, $[M+H]^+$ chemical formulas, and corresponding protonated masses of cannabinoids known to be in *Cannabis sativa* products.

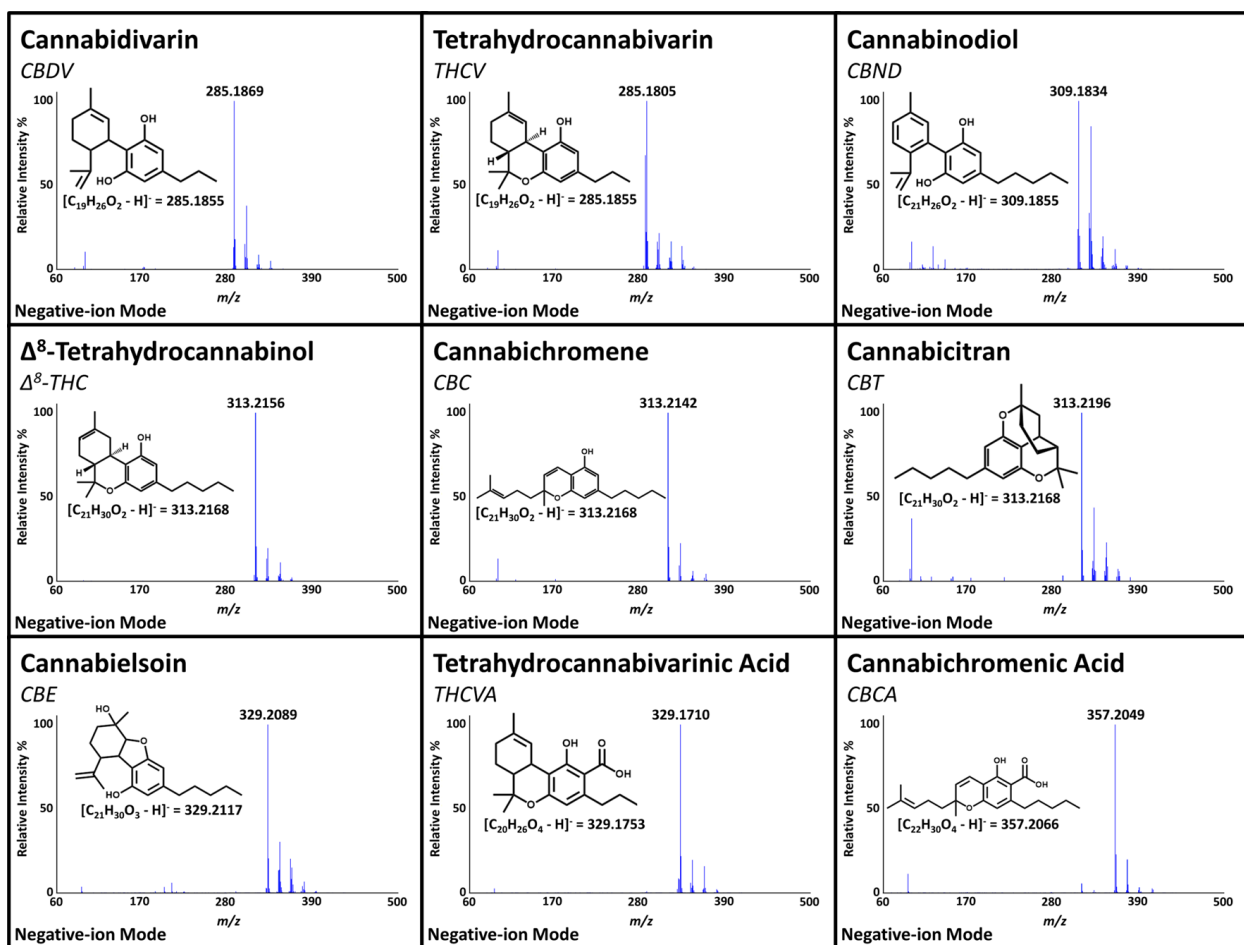


Figure S3. DART mass spectra (collected in negative-ion mode at an orifice 1 voltage of -20 V), structures, $[M-H]^-$ chemical formulas, and corresponding deprotonated masses of cannabinoids known to be in *Cannabis sativa* products.

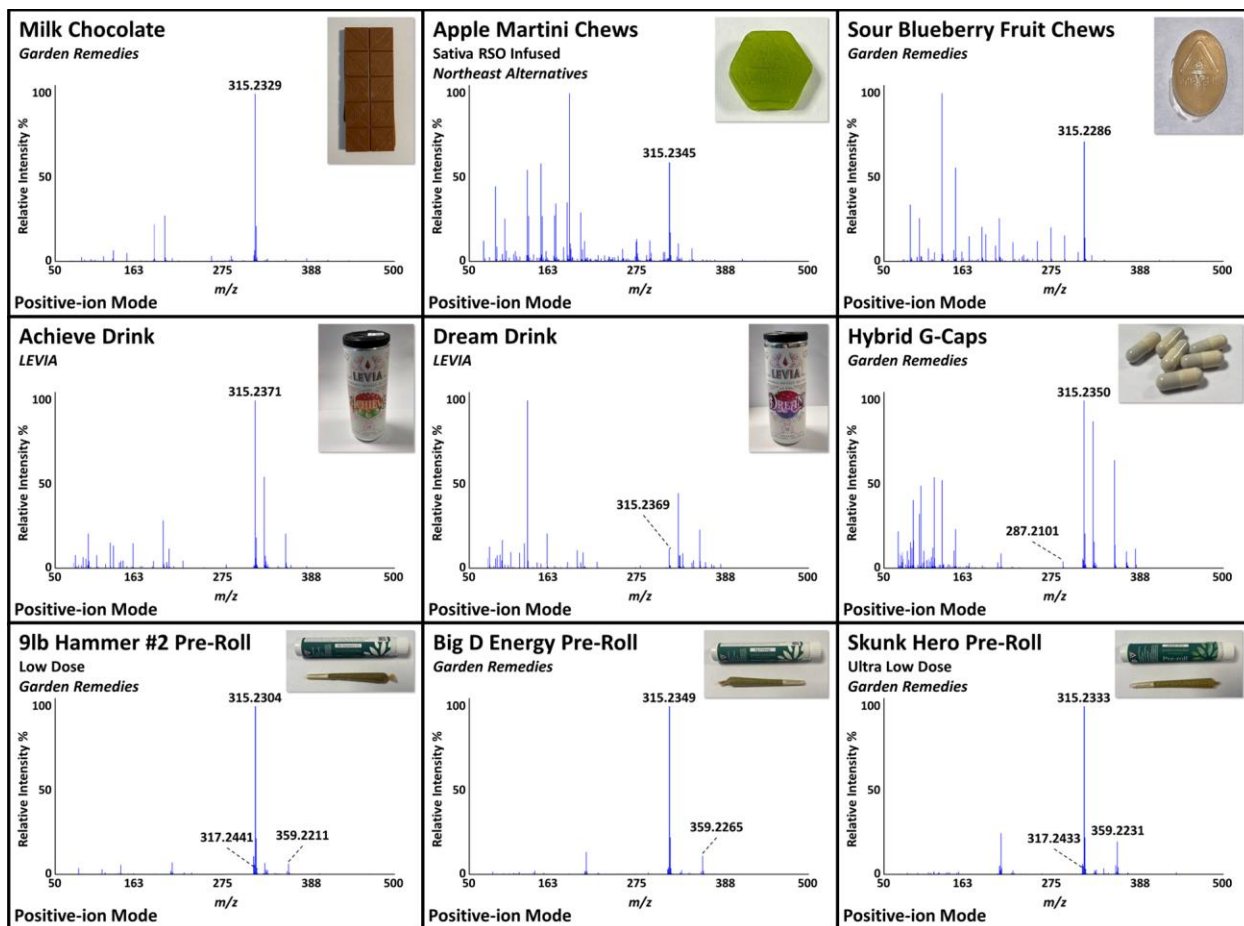


Figure S4. DART mass spectra (collected in positive-ion mode at an orifice 1 voltage of 20 V) of the remaining edibles, capsules, and pre-rolls not featured in **Figure 3** of the main document, with photographs of the products featured in the insets. Peaks consistent with reported cannabinoids are labeled, in addition to those with high relative intensities. Images of the corresponding products are shown in the insets.

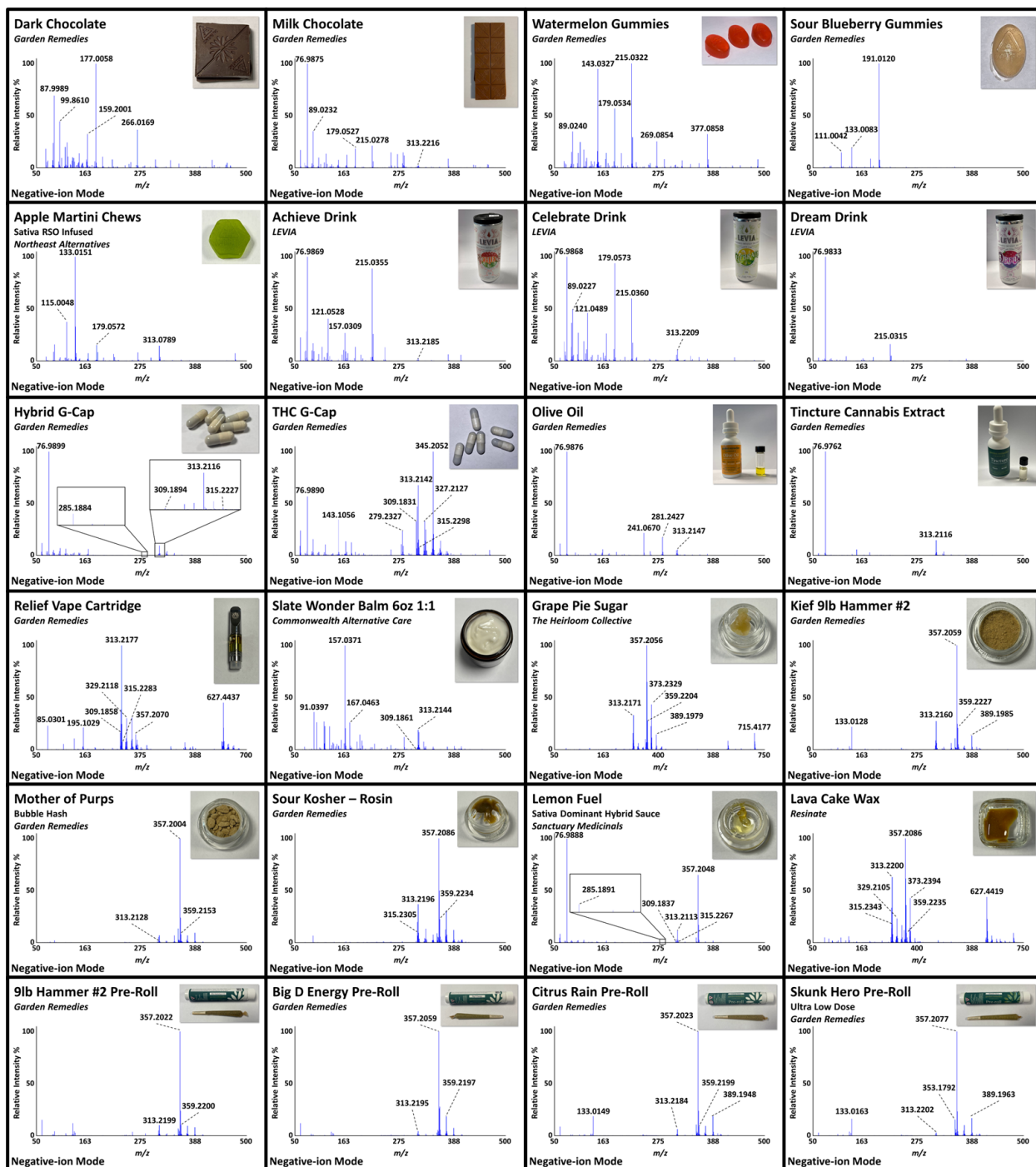


Figure S5. DART mass spectra (collected in negative-ion mode at an orifice 1 voltage of -20 V) for all non-flower *Cannabis* products (i.e., edibles, capsules, oils, tinctures, vape products, topicals, concentrates, and pre-rolls), with photographs of the products featured in the insets. Peaks consistent with reported cannabinoids are labeled, in addition to those with high relative intensities. Images of the corresponding products are shown in the insets.

Table S1. Detection of <i>m/z</i> values representing protonated masses consistent with cannabinoids and terpenes reported to be present in various recreational <i>Cannabis</i> products analyzed by DART-HRMS in positive-ion mode.								
Product Category	Product	Brand	M+H Det.	Protonated Formula	Molecules*	[M+H] ⁺ calc.	Diff. (mmu)	Int.
Edibles	Milk Chocolate Bar	Garden Remedies	315.2329	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	0.5	17307
	Dark Chocolate Bar	Garden Remedies	315.2362	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	3.8	4830
	Sour Blueberry Chew – 20 Pack	Garden Remedies	315.2286	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-3.8	4499
	Watermelon Chew – 20 Pack	Garden Remedies	315.2337	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	1.3	5217
	Apple Martini – Chew – RSO Sativa – 100MG – 20 Pack	Cannatini	315.2345	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	2.1	271281
	Achieve – Social Seltzer (12 oz) – 5 mg	Levia	315.2371	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	4.7	3109
	Celebrate – Social Seltzer (12oz) – 5 mg	Levia	315.2349	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	2.5	1748
	Dream – Social Seltzer (12oz) – 5 mg	Levia	315.2369	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	4.5	674
	1:1 – G-Caps – 20 Pack	Garden Remedies	287.2101	C ₁₉ H ₃₆ O ₂ + H ⁺	CBDV, THCV	287.2011	9.0	171
			315.2350	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBD, CBC, CBT	315.2324	2.6	4254
	THC – G-Caps – 20 Pack	Garden Remedies	315.2338	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBC	315.2324	1.4	1835
Infused Olive Oil	Garden Remedies	315.2340	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	1.6	7530	
Concentrates	Sour Kosher – Rosin 1g	Garden Remedies	315.2309	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBT	315.2324	-1.5	71474
			359.2233	C ₂₂ H ₃₀ O ₄ + H ⁺	CBDA, THCA, CBCA	359.2222	1.1	2646
	Lava Cake Wax	Resinate	315.2348	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBC	315.2324	2.4	189230
			317.2425	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-5.6	21376
			359.2227	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA, CBDA	359.2222	0.5	4201
			361.2379	C ₂₂ H ₃₂ O ₄ + H ⁺	CBGA	361.2379	0.2	456
	9lb Hammer #2 – Kief 1g	Garden Remedies	315.2316	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-0.8	8125
			359.2242	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	2.0	726
	Grape Pie – Sugar	The Heirloom Collective	315.2370	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	4.6	174375
			359.2240	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	1.8	27769
			361.2346	C ₂₂ H ₃₂ O ₄ + H ⁺	CBGA	361.2379	-3.3	1422
	Lemon Fuel – Sativa Dominant Hybrid – Sauce	Sanctuary Medicinals	315.2322	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBD, Δ ⁸ -THC, CBT	315.2324	-0.2	23395
			317.2453	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-2.8	766
			359.2242	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	2.0	473
Mother of Purps – Bubble Hash	Garden Remedies	315.2362	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	3.8	8277	
		317.2463	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-1.8	215	
		359.2272	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA, CBCA	359.2222	5.0	279	
Tinctures	CBD Tincture	Garden Remedies	315.2341	C ₂₁ H ₃₀ O ₂ + H ⁺	CBD	315.2324	1.7	1511
Topicals	Slate Wonder Balm – 6oz (1:1)	Commonwealth Alternative Care	311.2099	C ₂₁ H ₂₆ O ₂ + H ⁺	CBN	311.2011	8.8	388
			315.2355	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBD	315.2324	3.1	112379
			317.2466	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-1.5	4652

Table S1 continued. Detection of *m/z* values representing protonated masses consistent with cannabinoids and terpenes reported to be present in various recreational *Cannabis* products analyzed by DART-HRMS in positive-ion mode.

Product Category	Product	Brand	M+H Det.	Protonated Formula	Molecules*	[M+H] ⁺ calc.	Diff. (mmu)	Int.
Vaporizers	Relief – Vape	Garden Remedies	135.1122	C ₁₀ H ₁₄ + H ⁺	Para cymene	135.1174	-5.2	4089
			137.1320	C ₁₀ H ₁₆ + H ⁺	α-pinene, camphene, β-myrcene, β-pinene, Δ ³ -carene, α-terpinene, ocimene, Δ-limonene, β-ocimene, γ-terpinene, terpinolene	137.1330	-1.0	12888
			205.1962	C ₁₅ H ₂₄ + H ⁺	β-caryophyllene, α-humulene	205.1956	0.6	32620
			221.1910	C ₁₅ H ₂₄ O + H ⁺	Caryophyllene oxide	221.1905	0.5	6866
			287.2026	C ₁₉ H ₂₆ O ₂ + H ⁺	THCV	287.2011	1.5	6069
			311.2024	C ₂₁ H ₂₆ O ₂ + H ⁺	CBN	311.2011	1.3	4662
			315.2350	C ₂₁ H ₃₀ O ₂ + H ⁺	THC, CBD, CBC, CBT	315.2324	2.6	215246
			317.2419	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-6.2	17540
Pre-Rolls	9lb Hammer #2 Pre-Roll (Low Dose)	Garden Remedies	315.2304	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-2.0	7511
			317.2441	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-4.0	193
			359.2211	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	-1.1	478
	Big D Energy Pre-Roll	Garden Remedies	315.2349	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	2.5	15822
			359.2265	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	4.3	1735
			315.2317	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-0.7	10639
	Citrus Rain Pre-Roll	Garden Remedies	317.2490	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	0.9	259
			359.2220	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA, CBCA	359.2222	-0.2	1144
			315.2333	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	0.9	12196
	Skunk Hero Pre-Roll	Garden Remedies	317.2433	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-4.8	308
			359.2231	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA, CBCA	359.2222	0.9	2383
			137.1328	C ₁₀ H ₁₆ + H ⁺	β-myrcene, β-pinene, limonene	137.1330	-0.2	94
Flower	Snowdog (Hybrid Strain)	Berkshire Roots	205.1984	C ₁₅ H ₂₄ + H ⁺	β-caryophyllene, α-humulene	205.1956	2.8	267
			315.2305	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-1.9	2614
			359.2254	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	3.2	600
			135.1208	C ₁₀ H ₁₄ + H ⁺	Para cymene	135.1174	3.4	41
	Dr. Lime #10 – Growers Reserve Flower (Sativa Strain)	Garden Remedies	137.1351	C ₁₀ H ₁₆ + H ⁺	β-myrcene, limonene, ocimene, β-pinene, α-pinene, terpinolene, camphene, terpinene	137.1330	2.1	122
			205.1963	C ₁₅ H ₂₄ + H ⁺	β-caryophyllene, humulene	205.1956	0.7	478
			221.1953	C ₁₅ H ₂₄ O + H ⁺	Caryophyllene oxide	221.1905	4.8	41
			315.2288	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-3.6	7128
			317.2471	C ₂₁ H ₃₂ O ₂ + H ⁺	CBG	317.2481	-1.0	186
			359.2231	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA, CBCA	359.2222	0.9	1104
			137.1328	C ₁₀ H ₁₆ + H ⁺	α-pinene, β-pinene, β-myrcene, limonene, terpinolene	137.1330	-0.2	94
	Wonka Bars (Indica Strain)	Nature's Heritage	205.1984	C ₁₅ H ₂₄ + H ⁺	β-caryophyllene, humulene	205.1956	2.8	267
			315.2305	C ₂₁ H ₃₀ O ₂ + H ⁺	THC	315.2324	-1.9	2614
			359.2254	C ₂₂ H ₃₀ O ₄ + H ⁺	THCA	359.2222	3.2	600

*Compound identities are tentatively assigned based on calculated/measured masses, and compounds reported as present on product labels.

Table S2. Detection of m/z values consistent with the protonated masses of cannabinoids reported in various recreational <i>Cannabis</i> products analyzed by DART-HRMS in negative-ion mode.								
Product Category	Product	Brand	M-H Det.	Deprotonated Formula	Molecules*	[M-H] ⁺ calc.	Diff. (mmu)	Int.
Edibles	Milk Chocolate Bar	Garden Remedies	313.2216	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	4.8	692
	Achieve – Social Seltzer (12 oz) – 5 mg	Levia	313.2185	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	1.7	785
	Celebrate – Social Seltzer (12oz) – 5 mg	Levia	313.2209	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	4.1	2856
	1:1 – G-Caps – 20 Pack	Garden Remedies	285.1884	C ₁₉ H ₂₆ O ₂ - H ⁻	CBDV, THCV	285.1855	2.9	193
			309.1894	C ₂₁ H ₂₆ O ₂ - H ⁻	CBN	309.1855	3.9	175
			313.2116	C ₂₁ H ₃₀ O ₂ - H ⁻	CBD, THC, CBC, CBT	313.2168	-5.2	5535
	THC – G-Caps – 20 Pack	Garden Remedies	315.2227	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-9.7	273
			309.1831	C ₂₁ H ₂₆ O ₂ - H ⁻	CBN	309.1855	-2.4	10738
			313.2142	C ₂₁ H ₃₀ O ₂ - H ⁻	THC, CBC	313.2168	-2.6	22275
	Infused Olive Oil	Garden Remedies	315.2298	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-2.6	2490
313.2147			C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	-2.1	2560	
Concentrates	Sour Kosher – Rosin 1g	Garden Remedies	313.2196	C ₂₁ H ₃₀ O ₂ - H ⁻	THC, CBT	313.2168	2.8	82076
			315.2305	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-1.9	8421
			357.2086	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA, CBDA, CBCA	357.2066	2.0	222767
			359.2234	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	1.2	50030
	Lava Cake Wax	Resinate	313.2200	C ₂₁ H ₃₀ O ₂ - H ⁻	THC, CBC	313.2168	3.2	94744
			315.2343	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	1.9	12069
			357.2086	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA, CBDA	357.2066	2.0	150513
			359.2235	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	1.3	54313
	9lb Hammer #2 – Kief 1g	Garden Remedies	313.2160	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	-0.8	4337
			357.2059	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-0.7	15849
			359.2227	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	0.5	3326
	Grape Pie – Sugar	The Heirloom Collective	313.2171	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	0.3	53170
			357.2056	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-1.0	161346
			359.2204	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-1.8	45217
	Lemon Fuel – Sativa Dominant Hybrid – Sauce	Sanctuary Medicinals	285.1891	C ₁₉ H ₂₆ O ₂ - H ⁻	THCV	285.1855	3.6	115
			309.1837	C ₂₁ H ₂₆ O ₂ - H ⁻	CBN	309.1855	-1.8	1251
			313.2113	C ₂₁ H ₃₀ O ₂ - H ⁻	CBD, THC, Δ ⁸ -THC, CBT	313.2168	-3.6	6887
			315.2267	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-5.7	635
			357.2048	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-1.8	38647
	Mother of Purps – Bubble Hash	Garden Remedies	313.2128	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	4.0	929
357.2004			C ₂₂ H ₃₀ O ₄ - H ⁻	THCA, CBCA	357.2066	-6.2	11277	
359.2153			C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-6.9	920	
Tinctures	CBD Tincture	Garden Remedies	313.2116	C ₂₁ H ₃₀ O ₂ - H ⁻	CBD	313.2168	-5.2	13299
Topicals	Slate Wonder Balm – 6oz (1:1)	Commonwealth Alternative Care	309.1861	C ₂₁ H ₂₆ O ₂ - H ⁻	CBN	309.1855	0.6	3895
			313.2144	C ₂₁ H ₃₀ O ₂ - H ⁻	THC, CBD	313.2168	-2.4	67662
Vaporizers	Relief – Vape	Garden Remedies	309.1858	C ₂₁ H ₂₆ O ₂ - H ⁻	CBN	309.1855	0.3	20942
			313.2177	C ₂₁ H ₃₀ O ₂ - H ⁻	THC, CBD, CBC, CBT	313.2168	0.9	129682
			315.2283	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-4.1	9713
			357.2070	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	0.4	19182

Table S2 continued. Detection of m/z values consistent with the protonated masses of cannabinoids reported in various recreational *Cannabis* products analyzed by DART-HRMS in negative-ion mode.

Product Category	Product	Brand	M-H Det.	Deprotonated Formula	Molecules*	[M-H] ⁻ calc.	Diff. (mmu)	Int.
Pre-Rolls	9lb Hammer #2 Pre-Roll (Low Dose)	Garden Remedies	313.2199	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	3.1	1185
			357.2022	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-4.4	11598
			359.2200	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-2.2	1201
	Big D Energy Pre-Roll	Garden Remedies	313.2195	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	2.7	715
			357.2059	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-0.7	16371
			359.2197	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-2.5	4564
	Citrus Rain Pre-Roll	Garden Remedies	313.2184	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	1.6	969
			357.2023	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA, CBCA	357.2066	-4.3	15627
			359.2199	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-2.3	1387
	Skunk Hero Pre-Roll	Garden Remedies	313.2202	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	3.4	388
			357.2077	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA, CBCA	357.2066	1.1	12708
	Flower	Snowdog (Hybrid Strain)	Berkshire Roots	313.2173	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	0.5
315.2284				C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-4.0	299
357.2061				C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-0.5	47792
Dr. Lime #10 – Growers Reserve Flower (Sativa Strain)		Garden Remedies	313.2191	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	2.3	516
			357.2069	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA, CBCA	357.2066	0.3	3694
			359.2218	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-0.4	210
Wonka Bars (Indica Strain)		Nature's Heritage	313.2168	C ₂₁ H ₃₀ O ₂ - H ⁻	THC	313.2168	0.0	4298
			315.2243	C ₂₁ H ₃₂ O ₂ - H ⁻	CBG	315.2324	-8.1	322
			357.2054	C ₂₂ H ₃₀ O ₄ - H ⁻	THCA	357.2066	-1.2	46625
			359.2128	C ₂₂ H ₃₂ O ₄ - H ⁻	CBGA	359.2222	-9.4	3491

*Compound identities are tentatively assigned based on calculated/measured masses, and compounds reported as present on product labels.

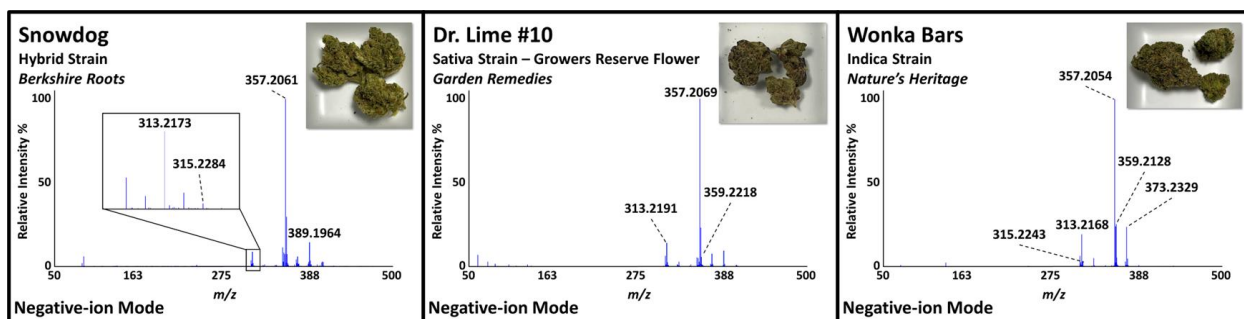


Figure S6. DART mass spectra (collected in negative-ion mode at an orifice 1 voltage of -20 V) of the recreational *Cannabis* flower samples, with photographs of the flower shown in the insets. Peaks consistent with reported cannabinoids are labeled. Images of the corresponding products are shown in the insets.

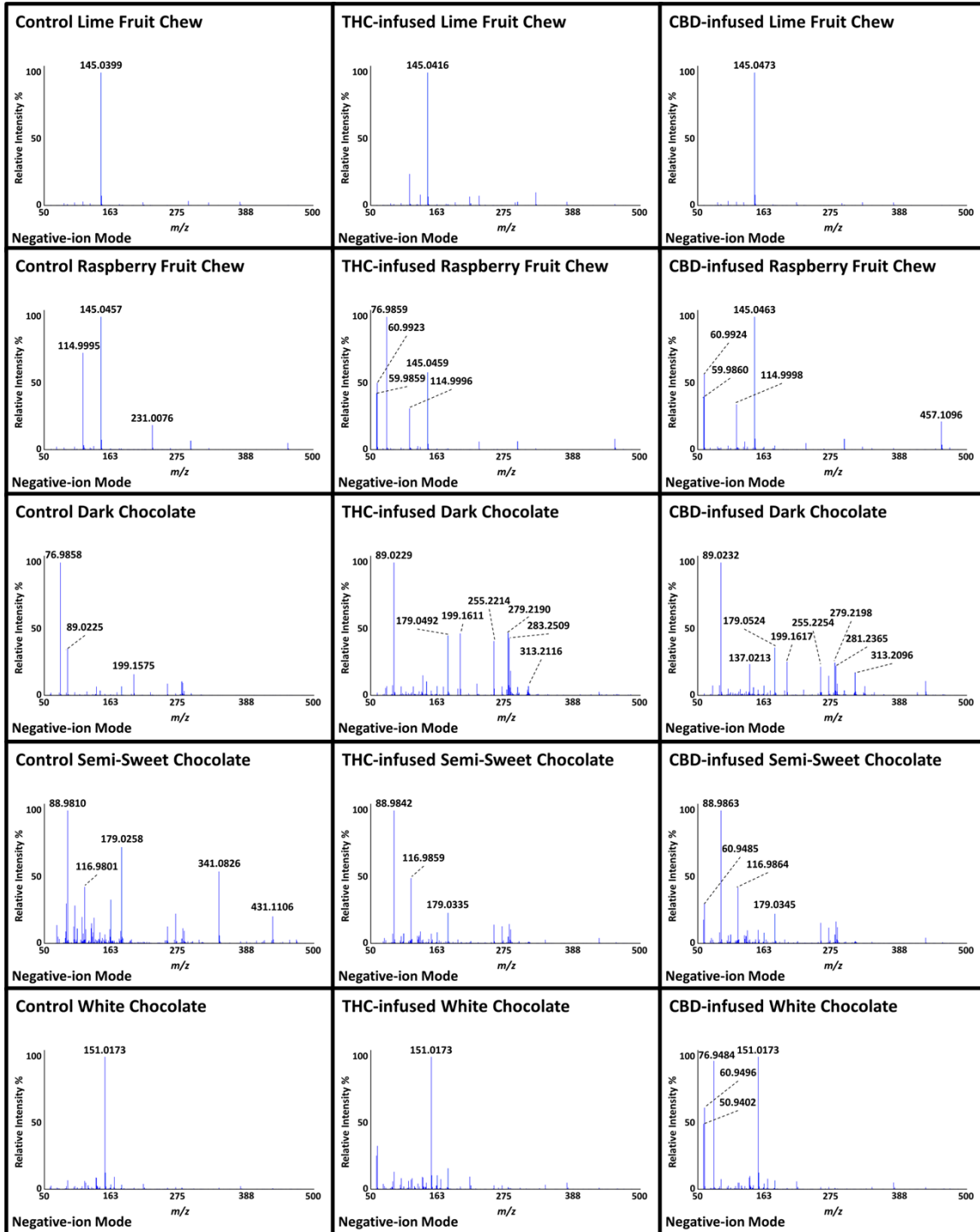


Figure S7. DART mass spectra (collected in negative-ion mode at an orifice 1 voltage of -20 V) of the edible candies prepared in-house from our previous study. Only the THC- and CBD-infused dark chocolates produced peaks within 10 mmu of the mass consistent with deprotonated THC/CBD.